

(+)-«gamma»-Gurjunene

Inchi:

InChI=1S/C15H24/c1-10(2)13-7-5-11(3)14-8-6-12(4)15(14)9-13/h9,11-14H,1,5-8H2,2-4H

InchiKey:

DUYRYUZIBGFLDD-AAVRWANBSA-N

Formula:

C15H24

SMILES:

C=C(C)C1C=C2C(C)CCC2C(C)CC1

Mol. weight [g/mol]:

204.35

Physical Properties

Property code	Value	Unit	Source
gf	232.72	kJ/mol	Joback Method
hf	-110.70	kJ/mol	Joback Method
hfus	22.86	kJ/mol	Joback Method
hvap	49.24	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.581		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1896.95	kPa	Joback Method
rinpol	1479.00		NIST Webbook
tb	564.52	K	Joback Method
tc	780.55	K	Joback Method
tf	269.69	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.34	J/mol×K	564.52	Joback Method
cpg	525.40	J/mol×K	600.53	Joback Method
cpg	548.06	J/mol×K	636.53	Joback Method
cpg	569.37	J/mol×K	672.54	Joback Method
cpg	589.37	J/mol×K	708.54	Joback Method
cpg	608.13	J/mol×K	744.55	Joback Method
cpg	625.69	J/mol×K	780.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R336706&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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